



# Viewing 2C07\_cyclopentadieneFH-multi.table

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All-Atom Contacts	Clashscore, all atoms:	2.38		99 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	236	97.52%	Goal: >98%
	MolProbity score^	1.12		100 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 982	0.00%	Goal: 0%
	Bad backbone angles:	1 / 1224	0.08%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.

\* 100<sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

<sup>^</sup> MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg:	Clashscore:	Outliers: 0 of	Poor rotamers: 0	Outliers:	Outliers:	Outliers: 1 of
		33.75	2.38	242	of 209	0 of 224	0 of 246	246
A 2	SO4	28.36	-	-	-	-	-	-
A 54	LYS	48.37	0.503Å N with A2008 HOH O	-	98.6% ( <i>mttt</i> ) chi angles: 290.4,185,177.2,175.7	0.008Å	-	-
A 55	GLU	43.08	-	Favored (34.15%) General case / -145.1,163.5	15.5% ( <i>pt-20</i> ) chi angles: 68.4,195.8,147.8	0.061Å	-	-
A 56	ASN	26.37	-	Favored (28.77%) General case / -78.6,157.0	77.5% ( <i>m-20</i> ) chi angles: 288.9,354.7	0.138Å	-	-
A 57	TYR	48.12	-	Favored (51.57%) General case / -122.0,128.5	61% ( <i>t80</i> ) chi angles: 173.1,67.4	0.104Å	-	-

A 58	TYR	24.94	-	Favored (16.75%) General case / -109.6,106.9	76.3% ( <i>m-85</i> ) chi angles: 299.8,109	0.036Å	-	-
A 59	TYR	30.51	-	Favored (21.43%) General case / -79.5,118.5	56% ( <i>t80</i> ) chi angles: 174.3,64.9	0.037Å	-	-
A 60	CYS	24.36	-	Favored (28.12%) General case / -107.8,11.5	96% ( <i>m</i> ) chi angles: 294	0.016Å	-	-
A 61	GLY	29.06	-	Favored (29.69%) Glycine / 100.4,179.8	-	-	-	-
A 62	GLU	41.97	-	Favored (31.43%) General case / -100.0,142.5	62.4% ( <i>mm-40</i> ) chi angles: 306.4,296.2,133.9	0.051Å	-	-
A 63	ASN	41.92	-	Favored (30.16%) General case / 53.7,39.4	70.2% ( <i>m-80</i> ) chi angles: 303.4,299.8	0.032Å	-	-
A 64	LYS	33.77	-	Favored (23.95%) General case / -89.0,148.1	74% ( <i>mmtt</i> ) chi angles: 303,294.7,180.8,189.5	0.017Å	-	-
A 65	VAL	26.95	-	Favored (74.58%) Isoleucine or valine / -119.5,130.0	73% ( <i>t</i> ) chi angles: 173.9	0.084Å	-	-
A 66	ALA	22.32	-	Favored (29.33%) General case / -113.5,153.0	-	0.065Å	-	-
A 67	LEU	31.67	-	Favored (25.91%) General case / -135.0,125.1	18.6% ( <i>tp</i> ) chi angles: 170.2,52.2	0.071Å	-	-
A 68	VAL	20.22	-	Favored (66.26%) Isoleucine or valine / -121.2,122.0	48.7% ( <i>t</i> ) chi angles: 182.7	0.066Å	-	-
A 69	THR	21.57	0.412Å O with A 147 ASN HB3	Favored (18.58%) General case / -90.8,155.7	43.6% ( <i>p</i> ) chi angles: 67.1	0.053Å	-	-

A 70	GLY	23.11	-	Favored (94.12%) Glycine / 59.6,38.7	-	-	-	-
A 71	ALA	23.61	-	Favored (45.65%) General case / -82.1,-0.7	-	0.031Å	-	-
A 72	GLY	28.11	-	Favored (76.89%) Glycine / -71.9,-24.2	-	-	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 73	ARG	58.01	0.407Å HB3 with A 73 ARGNH1	Favored (23.91%) General case / -156.9,169.8	2.4% ( <i>ptp180</i> ) chi angles: 63.6,198.6,83.2,272.3	0.095Å	-	-
A 74	GLY	24.45	-	Favored (44.93%) Glycine / 54.2,-134.2	-	-	-	-
A 75	ILE	23.15	-	Favored (81.4%) Isoleucine or valine / -56.7,-48.1	91.5% ( <i>mt</i> ) chi angles: 291.5,168.5	0.058Å	-	-
A 76	GLY	19.59	-	Favored (94.2%) Glycine / -57.6,-43.7	-	-	-	-
A 77	ARG	42.5	-	Favored (97.03%) General case / -64.0,-43.0	15.2% ( <i>ttt180</i> ) chi angles: 181.6,164.2,191.3,127.7	0.032Å	-	-
A 78	GLU	37.95	-	Favored (73.8%) General case / -68.9,-33.5	68.4% ( <i>mm-40</i> ) chi angles: 294.3,309.6,129.3	0.033Å	-	-
A 79	ILE	20.77	-	Favored (89.71%) Isoleucine or valine / -65.8,-46.1	67.2% ( <i>mt</i> ) chi angles: 289.5,175.6	0.019Å	-	-
A 80	ALA	21.65	-	Favored (99.78%) General case / -62.8,-42.6	-	0.028Å	-	-
				Favored (96.05%)	48.7% ( <i>mtpt</i> )			

A 81	LYS	33.35	-	General case / -64.4,-42.6	chi angles: 287.7,158.9,59.6,186.2	0.015Å	-	-
A 82	MET	25.64	-	Favored (71.06%) General case / -71.6,-37.4	43.5% ( <i>ttm</i> ) chi angles: 197,172.4,286.5	0.007Å	-	-
A 83	LEU	23.62	-	Favored (72.87%) General case / -62.0,-32.4	35.1% ( <i>mt</i> ) chi angles: 281.1,173.3	0.04Å	-	-
A 84	ALA	30.27	-	Favored (63.51%) General case / -59.5,-24.2	-	0.022Å	-	-
A 85	LYS	49.03	-	Favored (64.06%) General case / -69.0,-22.0	53.2% ( <i>mtpt</i> ) chi angles: 300.1,160.8,66.7,174.5	0.014Å	-	-
A 86	SER	37.04	-	Favored (3.53%) General case / -134.7,7.5	10.7% ( <i>p</i> ) chi angles: 46.5	0.16Å	-	-
A 87	VAL	33.12	-	Favored (13.69%) Isoleucine or valine / -114.4,160.6	21.4% ( <i>m</i> ) chi angles: 303.2	0.027Å	-	-
A 88	SER	39.77	-	Favored (62.9%) General case / -74.3,-32.5	98.5% ( <i>p</i> ) chi angles: 64.6	0.05Å	-	-
A 89	HIS	31.84	-	Favored (15.19%) General case / -150.9,132.9	15.9% ( <i>t60</i> ) chi angles: 190.6,100.9	0.064Å	-	-
A 90	VAL	26.33	-	Favored (62%) Isoleucine or valine / -116.2,119.5	78.1% ( <i>t</i> ) chi angles: 174.3	0.065Å	-	-
A 91	ILE	23.2	-	Favored (43.68%) Isoleucine or valine / -95.5,130.9	66.2% ( <i>mt</i> ) chi angles: 304.5,170.8	0.072Å	-	-
A 92	CYS	25.69	-	Favored (55.78%) General case / -112.0,130.7	73.4% ( <i>m</i> ) chi angles: 296.9	0.081Å	-	-

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
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			Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 93	ILE	26.05	-	Favored (67.47%) Isoleucine or valine / -118.3,132.7	39.3% ( <i>mt</i> ) chi angles: 290.5,183	0.049Å	-	-	
A 94	SER	27.11	-	Favored (39.7%) General case / -139.2,160.5	66.3% ( <i>m</i> ) chi angles: 296.5	0.104Å	-	-	
A 95	ARG	51.89	-	Favored (84.64%) General case / -59.0,-40.4	70.6% ( <i>ttp85</i> ) chi angles: 187.5,175.8,65.6,75.5	0.02Å	-	-	
A 96	THR	32.79	-	Favored (36.87%) General case / -114.1,148.6	29.9% ( <i>p</i> ) chi angles: 70.4	0.057Å	-	-	
A 97	GLN	30.89	-	Favored (72.19%) General case / -61.5,-32.2	70.4% ( <i>tp60</i> ) chi angles: 190.4,65.5,49.8	0.026Å	-	-	
A 98	LYS	39.83	-	Favored (98.24%) General case / -62.2,-43.7	81.7% ( <i>tttt</i> ) chi angles: 170.1,183.5,178.9,180.1	0.045Å	-	-	
A 99	SER	34.26	-	Favored (88.56%) General case / -63.0,-46.2	19.4% ( <i>m</i> ) chi angles: 284.3	0.021Å	-	-	
A 100	CYS	34.63	-	Favored (63.36%) General case / -73.5,-30.8	16.9% ( <i>p</i> ) chi angles: 53.9	0.105Å	-	-	
A 101	ASP	37.92	-	Favored (74.61%) General case / -61.5,-33.9	99.6% ( <i>m-20</i> ) chi angles: 287.4,167.3	0.069Å	-	-	
A 102	SER	37.25	-	Favored (86.25%) General case / -62.5,-46.9	36.5% ( <i>t</i> ) chi angles: 175.9	0.022Å	-	-	
A 103	VAL	28.73	-	Favored (43.03%) Isoleucine or valine / -74.7,-37.4	7.3% ( <i>p</i> ) chi angles: 56.1	0.116Å	-	-	
Favored					61.9% ( <i>t</i> )				

A 104	VAL	28.57	-	Favored (81.26%) Isoleucine or valine / -60.3,-39.5	chi angles: 171.2	0.032Å	-	-
A 105	ASP	40.38	-	Favored (89.79%) General case / -66.3,-41.4	38.2% ( <i>m-20</i> ) chi angles: 277.5,7.1	0.059Å	-	-
A 106	GLU	40.92	-	Favored (95.85%) General case / -61.9,-44.9	79.9% ( <i>tt0</i> ) chi angles: 184.1,169.9,9.9	0.019Å	-	-
A 107	ILE	29.22	-	Favored (97.8%) Isoleucine or valine / -64.1,-44.8	94.5% ( <i>mt</i> ) chi angles: 292.2,170.2	0.032Å	-	-
A 108	LYS	49.86	-	Favored (72.16%) General case / -65.3,-31.2	98.2% ( <i>mttt</i> ) chi angles: 289.8,179.4,181.6,177.6	0.02Å	-	-
A 109	SER	43.85	-	Favored (55.77%) General case / -63.1,-15.2	69.2% ( <i>p</i> ) chi angles: 70.9	0.02Å	-	-
A 110	PHE	51.96	-	Favored (43.73%) General case / -100.5,8.1	44% ( <i>m-85</i> ) chi angles: 281.7,105.6	0.017Å	-	-
A 111	GLY	43	-	Favored (68.9%) Glycine / 88.8,9.1	-	-	-	-
A 112	TYR	40.69	-	Favored (11.22%) General case / -98.4,166.8	33% ( <i>m-85</i> ) chi angles: 302.5,125.6	0.021Å	-	-

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		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 113	GLU	45.9	-	Favored (40.8%) General case / -96.9,134.0	67.5% ( <i>mm-40</i> ) chi angles: 301.8,303.9,128.3	0.022Å	-	-
A 114	SER	31.19	-	Favored (18.81%) General case / -160.1,150.8	32.4% ( <i>t</i> ) chi angles: 184.2	0.023Å	-	-
				Favored				

A 115	SER	30.51	-	(45.38%) General case / -140.8,157.5 Favored	67.5% ( <i>p</i> ) chi angles: 57.3	0.009Å	-	-
A 116	GLY	28.8	-	(13.4%) Glycine / -134.7,142.0 Favored	-	-	-	-
A 117	TYR	38.27	-	(45.8%) General case / -128.8,129.6 Favored	23.4% ( <i>m</i> -85) chi angles: 298.9,71.6	0.085Å	-	-
A 118	ALA	28.25	-	(44.34%) General case / -74.2,139.3 Allowed	-	0.088Å	-	-
A 119	GLY	29.68	-	(1.08%) Glycine / -167.3,122.9 Favored	-	-	-	-
A 120	ASP	33.95	-	(17.4%) General case / -92.3,105.1 Favored	42.2% ( <i>t0</i> ) chi angles: 189.1,148.3	0.084Å	-	-
A 121	VAL	25.88	-	(16.25%) Isoleucine or valine / -62.8,-15.9 Favored	10.8% ( <i>m</i> ) chi angles: 308	0.059Å	-	-
A 122	SER	27.68	-	(58.24%) General case / -80.1,-6.8 Favored	53.4% ( <i>p</i> ) chi angles: 74.4	0.047Å	-	-
A 123	LYS	38.86	-	(9.62%) General case / -112.9,101.6 Favored	98.3% ( <i>mttt</i> ) chi angles: 297.6,182.1,177.8,177.5	0.078Å	-	-
A 124	LYS	49.58	-	(73.59%) General case / -55.7,-41.3 Favored	60.9% ( <i>pttt</i> ) chi angles: 58.2,180.5,175.7,183.1	0.099Å	-	-
A 125	GLU	45.69	-	(78.35%) General case / -68.5,-42.8 Favored	54% ( <i>mp0</i> ) chi angles: 293.6,87.6,172.2	0.009Å	-	-
A 126	GLU	36.93	-	(62.76%) General case / -64.8,-51.3 Favored	48.4% ( <i>tt0</i> ) chi angles: 180.4,180.7,135.3	0.022Å	-	-

A 127	ILE	27.14	-	(58.02%) Isoleucine or valine / -67.1,-32.5	10.3% ( <i>tp</i> ) chi angles: 197.5,66.5	0.106Å	-	-
A 128	SER	33.29	-	Favored (90.51%) General case / -62.8,-38.4	69.8% ( <i>m</i> ) chi angles: 293.2	0.035Å	-	-
A 129	GLU	49.18	-	Favored (78.16%) General case / -69.2,-37.6	17.5% ( <i>tp10</i> ) chi angles: 184,53.8,58.3	0.013Å	-	-
A 130	VAL	30.44	-	Favored (88.2%) Isoleucine or valine / -62.1,-48.5	59.4% ( <i>t</i> ) chi angles: 171	0.047Å	-	-
A 131	ILE	27.1	-	Favored (88.22%) Isoleucine or valine / -62.4,-40.5	45.3% ( <i>mm</i> ) chi angles: 297.9,296.9	0.024Å	-	-
A 132	ASN	47.76	0.59Å O with A 136 THR HG23	Favored (98.33%) General case / -61.5,-42.1	95.2% ( <i>m-20</i> ) chi angles: 285.7,338.7	0.033Å	-	-

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 133	LYS	52.81	-	Favored (95.75%) General case / -61.8,-45.0	82.3% ( <i>tttt</i> ) chi angles: 182.3,177.7,191.6,176.7	0.046Å	-	-
A 134	ILE	31.73	-	Favored (82.13%) Isoleucine or valine / -60.4,-39.8	73.5% ( <i>mt</i> ) chi angles: 288.9,172.6	0.055Å	-	-
A 135	LEU	32.75	-	Favored (59.96%) General case / -76.7,-12.2	57.3% ( <i>mt</i> ) chi angles: 291.2,182.8	0.068Å	-	-
A 136	THR	44.43	0.59Å HG23 with A 132 ASN O	Favored (24.35%) General case / -85.5,-29.3	45.1% ( <i>p</i> ) chi angles: 66.5	0.054Å	-	-
A 137	GLU	52.6	-	Favored (27%) General case / -83.7,-30.2	13.3% ( <i>tp10</i> ) chi angles: 169.2,79.8,165.2	0.032Å	-	-
				Favored (46.08%)	94.6% ( <i>m-70</i> )			



A 138	HIS	39.41	-	General case / -124.5,126.6	chi angles: 298.5,275.7	0.078Å	-	-
A 139	LYS	50.34	-	Favored (88.21%) General case / -64.8,-44.9	20.1% ( <i>tptm</i> ) chi angles: 166.9,56.8,179.4,298.6	0.065Å	-	-
A 140	ASN	39.95	-	Favored (50.19%) General case / -127.2,148.0	33.6% ( <i>m120</i> ) chi angles: 301,107.2	0.047Å	-	-
A 141	VAL	26.79	-	Favored (11.45%) Isoleucine or valine / -128.1,104.2	65.2% ( <i>t</i> ) chi angles: 171.4	0.07Å	-	OUTLIER(S) worst is N-CA-C: -4.768 &sigma;
A 142	ASP	25.37	-	Favored (35.38%) General case / -80.9,-29.7	23.3% ( <i>m-20</i> ) chi angles: 305.9,107.3	0.045Å	-	-
A 143	ILE	23.45	-	Favored (60.9%) Isoleucine or valine / -129.2,124.6	66.3% ( <i>mt</i> ) chi angles: 298.6,162.1	0.088Å	-	-
A 144	LEU	18.51	-	Favored (35.52%) General case / -123.1,121.2	28.6% ( <i>tp</i> ) chi angles: 167,63.5	0.065Å	-	-
A 145	VAL	18.55	-	Favored (21.81%) Isoleucine or valine / -110.5,107.0	59% ( <i>t</i> ) chi angles: 180.9	0.014Å	-	-
A 146	ASN	19.58	-	Favored (9.14%) General case / -86.1,93.9	64% ( <i>m-20</i> ) chi angles: 281.4,310.1	0.051Å	-	-
A 147	ASN	21.78	0.412Å HB3 with A 69 THR O	Favored (11.87%) General case / -111.7,-21.1	16% ( <i>t30</i> ) chi angles: 173.4,75.6	0.035Å	-	-
A 148	ALA	22.73	-	Favored (36.49%) General case / -53.6,137.8	-	0.024Å	-	-
A 149	GLY	23.94	-	Favored (27%) Glycine / -179.4,161.2	-	-	-	-
A 150	ILE	25.95	-	Favored (18.99%) Isoleucine or valine	40.1% ( <i>pt</i> ) chi angles: 56.7,169.9	0.141Å	-	-

/ -139.8,167.7

A 151	THR	27.18	-	Favored (48.15%) General case / -126.3,150.9	73.8% ( <i>p</i> ) chi angles: 59.9	0.086Å	-	-
A 152	ARG	35.99	-	Allowed (1.35%) General case / -147.9,75.5	89.4% ( <i>mmt-85</i> ) chi angles: 291.5,288.8,185.1,271.7	0.121Å	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 153	ASP	28.19	-	Favored (53.29%) General case / -69.2,145.3	69.2% ( <i>m-20</i> ) chi angles: 299.8,160.4	0.031Å	-	-
A 154	ASN	31.7	-	Allowed (0.18%) General case / 179.1,146.8	1.2% ( <i>m-20</i> ) chi angles: 241.7,329.1	0.088Å	-	-
A 155	LEU	30.1	-	Favored (47.2%) General case / -61.9,147.3	75.7% ( <i>mt</i> ) chi angles: 292.9,180.7	0.073Å	-	-
A 156	PHE	27.55	-	Favored (66.83%) General case / -53.6,-41.6	40.3% ( <i>t80</i> ) chi angles: 188.6,61.4	0.043Å	-	-
A 157	LEU	37.57	-	Favored (68.25%) General case / -57.1,-34.3	13.4% ( <i>mt</i> ) chi angles: 274.2,182.8	0.054Å	-	-
A 158	ARG	55.88	-	Favored (20.07%) General case / -97.7,-16.2	16.6% ( <i>mtp180</i> ) chi angles: 294.8,175.8,51.8,136.5	0.075Å	-	-
A 159	MET	24.44	-	Favored (43.2%) General case / -54.0,135.0	52.6% ( <i>ttn</i> ) chi angles: 186,170.4,289.6	0.026Å	-	-
A 160	LYS	51.1	-	Favored (21.85%) General case / -87.2,153.0	97.7% ( <i>mttt</i> ) chi angles: 297.1,175,185.4,174.1	0.046Å	-	-
				Favored (70.61%)	26.1% ( <i>m120</i> )			

A 161	ASN	45.58	-	General case / -57.5,-35.8	chi angles: 290.4,128.4	0.035Å	-	-
A 162	ASP	43.58	-	Favored (64.28%) General case / -71.5,-29.0	11.9% ( <i>p-10</i> ) chi angles: 58.8,119.6	0.046Å	-	-
A 163	GLU	27.91	-	Favored (78.8%) General case / -69.1,-38.0	86.1% ( <i>mt-10</i> ) chi angles: 296.5,178.4,147.5	0.032Å	-	-
A 164	TRP	22.92	-	Favored (13.43%) General case / -68.4,-55.0	59.2% ( <i>t-105</i> ) chi angles: 169.9,255.9	0.053Å	-	-
A 165	GLU	32.91	-	Favored (89.71%) General case / -59.8,-46.3	80.9% ( <i>mm-40</i> ) chi angles: 294,293.2,158.1	0.028Å	-	-
A 166	ASP	29.15	-	Favored (85.63%) General case / -62.9,-37.1	91.8% ( <i>m-20</i> ) chi angles: 290.9,169.4	0.026Å	-	-
A 167	VAL	20.48	-	Favored (69.73%) Isoleucine or valine / -71.7,-43.8	38.3% ( <i>t</i> ) chi angles: 165.9	0.077Å	-	-
A 168	LEU	23.91	-	Favored (90.57%) General case / -65.8,-42.6	39.6% ( <i>mt</i> ) chi angles: 282.5,174.1	0.036Å	-	-
A 169	ARG	27.05	-	Favored (89.39%) General case / -66.0,-42.7	33.3% ( <i>ttp-105</i> ) chi angles: 189.4,173.3,73,256.1	0.022Å	-	-
A 170	THR	23.71	-	Favored (58.25%) General case / -72.1,-46.0	59.2% ( <i>m</i> ) chi angles: 304.1	0.036Å	-	-
A 171	ASN	21.5	-	Favored (27.32%) General case / -85.2,-25.4	14.9% ( <i>m-20</i> ) chi angles: 300.4,5.4	0.025Å	-	-
A 172	LEU	20.26	-	Allowed (1.99%) General case / -120.5,-56.2	43.8% ( <i>tp</i> ) chi angles: 183.5,57	0.046Å	-	-

#    Res    **High B**    Clash > 0.4Å    **Ramachandran**    **Rotamer**    **Cβ deviation**    **Bond lengths.**    **Bond angles.**

			Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
					Favored (65.94%) General case / -56.6,-33.0	4.4% ( <i>m120</i> ) chi angles: 296.3,56	0.041Å	-	-
A 173	ASN	28.1		-	Favored (66.34%) General case / -58.8,-28.8	81.9% ( <i>p</i> ) chi angles: 60.6	0.075Å	-	-
A 175	LEU	27.89		-	Favored (70.19%) General case / -59.7,-32.1	95.8% ( <i>mt</i> ) chi angles: 295.3,176.5	0.031Å	-	-
A 176	PHE	38.03		-	Favored (69.39%) General case / -66.0,-49.0	66.9% ( <i>t80</i> ) chi angles: 187.7,76.6	0.042Å	-	-
A 177	TYR	30.41		-	Favored (71%) General case / -66.8,-30.7	60.2% ( <i>m-85</i> ) chi angles: 304.8,111.2	0.036Å	-	-
A 178	ILE	23.51		-	Favored (16.73%) Isoleucine or valine / -86.1,-46.8	67.9% ( <i>mt</i> ) chi angles: 294.3,161.1	0.063Å	-	-
A 179	THR	20.74		-	Favored (51.3%) General case / -77.9,-32.0	6.3% ( <i>m</i> ) chi angles: 315.7	0.031Å	-	-
A 180	GLN	28.05	0.45Å HB3 with A 181 PRO HD3		Favored (75.16%) Pre-proline / -60.9,-52.0	49.1% ( <i>tt0</i> ) chi angles: 190.3,184.2,54.4	0.09Å	-	-
A 181	PRO	27.94	0.45Å HD3 with A 180 GLN HB3		Favored (49.26%) Trans proline / -63.0,-38.1	49.6% ( <i>Cg_exo</i> ) chi angles: 336.9,37.2,83.8	0.051Å	-	-
A 182	ILE	25.99		-	Favored (83.94%) Isoleucine or valine / -68.4,-42.4	56% ( <i>mt</i> ) chi angles: 286.2,173	0.056Å	-	-
A 183	SER	23.88		-	Favored (71.69%) General case / -62.9,-30.7	54.6% ( <i>p</i> ) chi angles: 73.6	0.018Å	-	-
A 184	LYS	44.07		-	Favored (99.12%)	93.6% ( <i>mttt</i> ) chi angles:	0.018Å	-	-

				General case / -62.7,-41.3	286.3,179.1,173.3,171.2			
A 185	ARG	40.18	-	Favored (74.85%) General case / -69.9,-35.9	28.5% ( <i>mmt85</i> ) chi angles: 295.4,283.8,175.9,87.8	0.017Å	-	-
A 186	MET	21.98	-	Favored (90.54%) General case / -65.8,-39.1	48.2% ( <i>mtt</i> ) chi angles: 287,175.9,167.4	0.05Å	-	-
A 187	ILE	26.42	-	Favored (96.9%) Isoleucine or valine / -64.5,-43.9	46.6% ( <i>mt</i> ) chi angles: 284.7,164.2	0.064Å	-	-
A 188	ASN	44.49	-	Favored (83.76%) General case / -65.4,-36.4	27.2% ( <i>t-20</i> ) chi angles: 175.1,263	0.033Å	-	-
A 189	ASN	32.79	-	Favored (58.68%) General case / -86.7,-7.0	57.6% ( <i>t30</i> ) chi angles: 196.2,46.5	0.016Å	-	-
A 190	ARG	34.94	-	Favored (24.66%) General case / 55.9,45.2	94.1% ( <i>mtt-85</i> ) chi angles: 292.3,181.3,187.3,265.9	0.08Å	-	-
A 191	TYR	23.03	-	Favored (3.88%) General case / -166.1,138.2	67.2% ( <i>t80</i> ) chi angles: 187.3,79.5	0.124Å	-	-
A 192	GLY	20.11	-	Favored (24.92%) Glycine / -175.6,158.0	-	-	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 193	ARG	20.57	-	Favored (9.41%) General case / -138.3,113.6	87.9% ( <i>mmt-85</i> ) chi angles: 290.2,288,184.9,275.9	0.1Å	-	-
A 194	ILE	18.39	-	Favored (66.31%) Isoleucine or valine / -115.5,121.0	96.9% ( <i>mt</i> ) chi angles: 293.6,169	0.043Å	-	-
				Favored				

A 195	ILE	27.55	-	(53.3%)	43.1% ( <i>mt</i> )	0.049Å	-	-
				Isoleucine or valine chi angles: 295.6,155.6 / -120.7,117.5				
				Favored				
A 196	ASN	17.65	-	(51.66%)	84.2% ( <i>m-20</i> )	0.048Å	-	-
				General case / chi angles: 299,319.4				
				-104.6,126.4				
				Favored				
A 197	ILE	22.17	-	(37.32%)	48.5% ( <i>mm</i> )	0.058Å	-	-
				Isoleucine or valine chi angles: 304.3,301.5				
				/ -86.4,121.3				
				Allowed				
A 198	SER	19.35	0.453Å HA with A 216 LYS HD2	(0.36%)	40.8% ( <i>t</i> )	0.115Å	-	-
				General case / chi angles: 177				
				-109.4,-136.0				
				Favored				
A 199	SER	17.81	-	(5.61%)	29.7% ( <i>t</i> )	0.173Å	-	-
				General case / chi angles: 172.7				
				-168.9,153.2				
				Favored				
A 200	ILE	23.95	0.644Å CD1B with A 302 LEU HD23	(40.43%)	8.4% ( <i>tp</i> )	0.033Å	-	-
				Isoleucine or valine chi angles: 184.9,69.7				
				/ -59.1,-29.0				
				Favored				
A 201	VAL	26.16	-	(35.3%)	79.5% ( <i>t</i> )	0.072Å	-	-
				Isoleucine or valine chi angles: 172.5				
				/ -61.3,-25.0				
				Favored				
A 202	GLY	22.84	-	(78.46%)	-	-	-	-
				Glycine / -73.1,-17.0				
				Favored				
A 203	LEU	24.46	-	(10.42%)	55.2% ( <i>mt</i> )	0.075Å	-	-
				General case / chi angles: 294.2,164.1				
				-99.6,-34.0				
				Favored				
A 204	THR	20.54	-	(13.65%)	49.9% ( <i>p</i> )	0.108Å	-	-
				General case / chi angles: 65.9				
				-111.4,-15.1				
				Favored				
A 205	GLY	20.13	-	(30.13%)	-	-	-	-
				Glycine / 78.5,166.6				
				Favored				
A 206	ASN	27.11	-	(9.36%)	65.4% ( <i>t30</i> )	0.042Å	-	-
				General case / chi angles: 189.9,33.2				
				-161.4,139.5				
				Favored				
A 207	VAL	23.23	-	(20.79%)	26.8% ( <i>t</i> )	0.088Å	-	-
				Isoleucine or valine chi angles: 164.6				

A 208	GLY	22.34	-	/ -58.2,129.9	-	-	-	-
				Favored (86.29%) Glycine / 85.6,3.4				
A 209	GLN	25.73	-	Favored (2.97%) General case / -134.6,40.4	57.9% ( <i>mt-30</i> ) chi angles: 298.9,196,296.5	0.031Å	-	-
				Favored (70.9%) General case / -59.8,-32.8				
A 210	ALA	19.01	-	Favored (21.78%) General case / -74.4,-49.7	20.3% ( <i>p-10</i> ) chi angles: 50.4,351.1	0.068Å	-	-
				Favored (81.26%) General case / -60.2,-48.5				
A 211	ASN	21.04	-	Favored (88.56%) General case / -58.4,-43.9	47.7% ( <i>t80</i> ) chi angles: 190.6,68.9	0.038Å	-	-
				Favored (94.62%) General case / -60.0,-44.4				
A 212	TYR	26.28	-	Favored (87.5%) General case / -65.9,-43.7	34% ( <i>p</i> ) chi angles: 77	0.045Å	-	-
				Favored (61.49%) General case / -74.1,-28.7				

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 213	SER	20.45	-	Favored (88.56%) General case / -58.4,-43.9	54.1% ( <i>p</i> ) chi angles: 73.9	0.026Å	-	-
				Favored (94.62%) General case / -60.0,-44.4				
A 214	SER	17.16	-	Favored (87.5%) General case / -65.9,-43.7	34% ( <i>p</i> ) chi angles: 77	0.045Å	-	-
				Favored (61.49%) General case / -74.1,-28.7				
A 215	SER	16.48	-	Favored (80.33%) General case / -68.7,-39.9	-	0.051Å	-	-
				Favored (92.14%) Glycine / -57.9,-39.8				

0.453Å  
HD2 with A 198  
SER HA

A 219	VAL	17.97	-	Favored (50.59%) Isoleucine or valine / -55.9,-38.1	60.9% ( <i>t</i> ) chi angles: 171.1	0.033Å	-	-
A 220	ILE	19.78	-	Favored (81.56%) Isoleucine or valine / -69.2,-42.7	96.8% ( <i>mt</i> ) chi angles: 292.6,169.5	0.102Å	-	-
A 221	GLY	18.42	-	Favored (95.54%) Glycine / -62.5,-38.0	-	-	-	-
A 222	PHE	19.48	-	Favored (77.17%) General case / -60.9,-49.5	89.7% ( <i>t80</i> ) chi angles: 178.1,74.5	0.113Å	-	-
A 223	THR	16.6	-	Favored (66.05%) General case / -53.9,-50.6	53.3% ( <i>m</i> ) chi angles: 295.6	0.071Å	-	-
A 224	LYS	25.82	-	Favored (88.75%) General case / -66.1,-38.6	68.4% ( <i>mttm</i> ) chi angles: 294,183,178.6,292.2	0.065Å	-	-
A 225	SER	22.37	-	Favored (76.42%) General case / -66.0,-46.8	26.5% ( <i>m</i> ) chi angles: 285.8	0.089Å	-	-
A 226	LEU	26.68	-	Favored (86.93%) General case / -64.0,-37.3	3.3% ( <i>mp</i> ) chi angles: 255,69.4	0.011Å	-	-
A 227	ALA	18.23	-	Favored (83.23%) General case / -57.7,-42.2	-	0.026Å	-	-
A 228	LYS	33.35	-	Favored (88.81%) General case / -64.3,-37.8	83.9% ( <i>mttt</i> ) chi angles: 286.9,175.5,168.5,192.8	0.019Å	-	-
A 229	GLU	25.11	-	Favored (40.88%) General case / -79.7,-30.6	79.4% ( <i>mt-10</i> ) chi angles: 293.7,186.6,15.7	0.062Å	-	-
A 230	LEU	21.85	-	Favored (17.56%) General case / -104.8,-10.2	50.5% ( <i>mt</i> ) chi angles: 308.1,180.9	0.013Å	-	-
				Favored				



A 231	ALA	22.33	-	(68.27%) General case / -58.0,-32.8 Favored	-	0.037Å	-	-
A 232	SER	24.86	-	(63.27%) General case / -68.1,-14.8	96.2% ( <i>p</i> ) chi angles: 66.7	0.015Å	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 233	ARG	34.23	-	Favored (10.98%) General case / -101.3,23.4	15.2% ( <i>mmt180</i> ) chi angles: 288.6,278.2,171.1,143.9	0.022Å	-	-
A 234	ASN	30.3	-	Favored (16.44%) General case / 61.8,35.9	47.4% ( <i>m-20</i> ) chi angles: 310.3,315.2	0.058Å	-	-
A 235	ILE	20.47	-	Favored (72.5%) Isoleucine or valine / -115.1,127.8	84.5% ( <i>mt</i> ) chi angles: 295.4,165.1	0.115Å	-	-
A 236	THR	17.94	-	Favored (30.77%) General case / -105.4,145.4	68.8% ( <i>p</i> ) chi angles: 62	0.073Å	-	-
A 237	VAL	16.3	-	Favored (30.33%) Isoleucine or valine / -131.5,116.0	17.6% ( <i>t</i> ) chi angles: 189.5	0.066Å	-	-
A 238	ASN	16.87	-	Favored (35.59%) General case / -139.2,162.2	71.7% ( <i>m-80</i> ) chi angles: 292,293.7	0.098Å	-	-
A 239	ALA	17.02	-	Favored (41.75%) General case / -122.2,150.8	-	0.054Å	-	-
A 240	ILE	17.73	-	Favored (68.72%) Isoleucine or valine / -115.2,131.0	76.9% ( <i>mt</i> ) chi angles: 293.5,176.6	0.074Å	-	-
A 241	ALA	17.9	-	Favored (36.17%) Pre-proline / -116.5,92.2	-	0.068Å	-	-

A 242	PRO	18.83	-	Favored (52.97%) Trans proline / -72.9,153.4	32.3% ( <i>Cg_exo</i> ) chi angles: 338.7,37.3,81.3	0.076Å	-	-
A 243	GLY	21.63	-	Favored (5.44%) Glycine / -91.8,-131.9	-	-	-	-
A 244	PHE	37.22	-	Favored (19.6%) General case / -85.5,111.0	69.8% ( <i>m-85</i> ) chi angles: 287.4,101.2	0.034Å	-	-
A 245	ILE	25.5	-	Favored (65.87%) Isoleucine or valine / -112.5,130.7	44.4% ( <i>mm</i> ) chi angles: 306.9,302.3	0.061Å	-	-
A 246	SER	37.89	-	Favored (56.69%) General case / -57.5,136.4	92.5% ( <i>p</i> ) chi angles: 66	0.055Å	-	-
A 247	SER	44.15	-	-	10.7% ( <i>t</i> ) chi angles: 164.6	0.035Å	-	-
A 253	ILE	62.67	-	-	49.8% ( <i>mm</i> ) chi angles: 301.7,297.5	0.032Å	-	-
A 254	SER	60.65	-	Favored (47.93%) General case / -67.7,151.0	78.5% ( <i>p</i> ) chi angles: 59.2	0.032Å	-	-
A 255	GLU	64.4	-	Favored (67.31%) General case / -58.3,-31.2	5.7% ( <i>mm-40</i> ) chi angles: 256.7,306,133.6	0.022Å	-	-
A 256	GLN	62.05	-	Favored (67.16%) General case / -72.5,-40.2	55.9% ( <i>tp60</i> ) chi angles: 183.3,60.1,29.2	0.025Å	-	-
A 257	ILE	56.09	-	Favored (51.21%) Isoleucine or valine / -71.7,-34.2	63.8% ( <i>mt</i> ) chi angles: 290.6,177.8	0.012Å	-	-

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		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 258	LYS	57.62	-	Favored (89.5%) General case / -66.4,-40.1	40.1% ( <i>ttmt</i> ) chi angles: 186.4,179.1,300.1,182.2	0.04Å	-	-

A 259	LYS	58.95	-	Favored (85.27%) General case / -66.5,-37.5	54.7% ( <i>mtmt</i> ) chi angles: 292.4,189.1,297.8,179.6	0.023Å	-	-
A 260	ASN	55.72	-	Favored (99.55%) General case / -62.2,-42.7	3.2% ( <i>m120</i> ) chi angles: 280.8,41	0.035Å	-	-
A 261	ILE	44.37	-	Favored (8.91%) Isoleucine or valine / -64.0,-58.1	77.7% ( <i>mt</i> ) chi angles: 289.4,170.6	0.05Å	-	-
A 262	ILE	42.89	-	Favored (17.47%) Isoleucine or valine / -53.0,-31.6	49.2% ( <i>mt</i> ) chi angles: 297.5,183.3	0.048Å	-	-
A 263	SER	40.68	-	Favored (62.05%) General case / -68.6,-13.0	69.9% ( <i>m</i> ) chi angles: 297.2	0.01Å	-	-
A 264	ASN	47.41	-	Favored (32.15%) General case / -100.3,-3.0	61.8% ( <i>m-80</i> ) chi angles: 285.2,288.6	0.026Å	-	-
A 265	ILE	29.13	-	Favored (65.12%) Pre-proline / -101.7,115.3	62.6% ( <i>mt</i> ) chi angles: 305.5,173.1	0.069Å	-	-
A 266	PRO	25.54	-	Favored (54.59%) Trans proline / -50.5,-40.7	23.3% ( <i>Cg_exo</i> ) chi angles: 324.5,46.1,81.6	0.051Å	-	-
A 267	ALA	25.56	-	Favored (63.85%) General case / -61.6,-20.8	-	0.02Å	-	-
A 268	GLY	29.47	-	Favored (73.15%) Glycine / 75.2,23.8	-	-	-	-
A 269	ARG	27.29	-	Favored (15.95%) General case / -166.8,166.0	46.2% ( <i>ptt85</i> ) chi angles: 61.5,166.8,176.2,95.8	0.128Å	-	-
A 270	MET	36.51	-	Favored (20.41%) General case / -84.3,161.6	74.8% ( <i>mtm</i> ) chi angles: 292.5,194.8,288.7	0.055Å	-	-
				Favored				

A 271	GLY	23.91	-	(47.08%) Glycine / -85.6,172.8	-	-	-	-
A 272	THR	24.62	-	Favored (44.55%) Pre-proline / -114.1,156.1	25.6% ( <i>p</i> ) chi angles: 71.7	0.078Å	-	-
A 273	PRO	26.37	-	Favored (54.51%) Trans proline / -65.5,-26.4	22.5% ( <i>Cg_endo</i> ) chi angles: 19.7,323.9,157.5	0.07Å	-	-
A 274	GLU	47.6	-	Favored (79.79%) General case / -66.5,-35.3	61.5% ( <i>mp0</i> ) chi angles: 292.1,80.1,5.2	0.022Å	-	-
A 275	GLU	23.34	-	Favored (87.94%) General case / -66.7,-41.5	64.3% ( <i>mt-10</i> ) chi angles: 285.5,174,136.3	0.034Å	-	-
A 276	VAL	19.26	-	Favored (86.49%) Isoleucine or valine / -65.5,-39.9	60.4% ( <i>t</i> ) chi angles: 181.6	0.038Å	-	-
A 277	ALA	20.56	-	Favored (85.9%) General case / -61.8,-37.8	-	0.019Å	-	-

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		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 278	ASN	24.86	-	Favored (89.91%) General case / -58.6,-44.7	10% ( <i>m-80</i> ) chi angles: 266.7,282.5	0.014Å	-	-
A 279	LEU	18.19	-	Favored (94.44%) General case / -64.9,-40.0	54.1% ( <i>tp</i> ) chi angles: 175.9,58.3	0.044Å	-	-
A 280	ALA	18.25	-	Favored (85.24%) General case / -66.6,-37.6	-	0.035Å	-	-
A 281	CYS	22.44	-	Favored (67%) General case / -72.3,-32.9	90.9% ( <i>m</i> ) chi angles: 289.8	0.026Å	-	-
A 282	PHE	20.22	-	Favored (93.15%) General case /	58.9% ( <i>t80</i> ) chi angles: 169.6,71.4	0.078Å	-	-

				-62.5,-45.4					
A 283	LEU	20.73	-	Favored (67.7%) General case / -65.7,-26.3	92.3% ( <i>mt</i> ) chi angles: 291.5,171.1	0.025Å	-	-	-
A 284	SER	22.77	-	Favored (59.48%) General case / -81.3,-10.9	49.4% ( <i>m</i> ) chi angles: 300.8	0.123Å	-	-	-
A 285	SER	24.25	-	Favored (24.79%) General case / -74.1,165.7	53.9% ( <i>p</i> ) chi angles: 74.1	0.102Å	-	-	-
A 286	ASP	31.98	-	Favored (93.49%) General case / -63.2,-39.0	34.7% ( <i>t70</i> ) chi angles: 180.6,58.4	0.07Å	-	-	-
A 287	LYS	47.54	-	Favored (10.81%) General case / -79.8,6.5	9.5% ( <i>mtpt</i> ) chi angles: 326,160.9,91.9,183.8	0.052Å	-	-	-
A 288	SER	25.7	-	Favored (16.21%) General case / -109.2,22.1	70.5% ( <i>m</i> ) chi angles: 297.4	0.039Å	-	-	-
A 289	GLY	18.57	-	Favored (60.96%) Glycine / -66.8,-13.2	-	-	-	-	-
A 290	TYR	19.93	-	Favored (46.26%) General case / -99.1,2.7	4.1% ( <i>t80</i> ) chi angles: 208.2,59.2	0.054Å	-	-	-
A 291	ILE	18.31	-	Favored (42.33%) Isoleucine or valine / -96.9,117.9	95.6% ( <i>mt</i> ) chi angles: 297.5,168.8	0.062Å	-	-	-
A 292	ASN	20.87	-	Favored (14.49%) General case / -152.4,133.9	6% ( <i>t-20</i> ) chi angles: 217,332.8	0.075Å	-	-	-
A 293	GLY	17.23	-	Favored (69.25%) Glycine / 74.8,25.6	-	-	-	-	-
A 294	ARG	25.39	-	Favored (12.82%) General case / -109.7,164.2	18.7% ( <i>mmm180</i> ) chi angles: 309.5,314.9,303.7,182.8	0.091Å	-	-	-
				Favored					

A 295	VAL	21.19	-	(58.24%) Isoleucine or valine / -119.2,118.7	46.3% ( <i>t</i> ) chi angles: 183.4	0.068Å	-	-
A 296	PHE	32.66	-	Favored (29.69%) General case / -106.5,115.1	7.7% ( <i>m-30</i> ) chi angles: 280.2,9.9	0.06Å	-	-
A 297	VAL	20.9	-	Favored (42.1%) Isoleucine or valine / -92.2,129.9	78.3% ( <i>t</i> ) chi angles: 174.3	0.092Å	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A 298	ILE	18.93	-	Favored (3.38%) Isoleucine or valine / -126.7,96.1	11.9% ( <i>tt</i> ) chi angles: 176.6,163.3	0.112Å	-	-
A 299	ASP	20.58	-	Allowed (1.49%) General case / -145.1,14.7	24.8% ( <i>p-I0</i> ) chi angles: 73.9,168.8	0.031Å	-	-
A 300	GLY	21.67	-	Favored (62.49%) Glycine / 62.8,20.8	-	-	-	-
A 301	GLY	26.74	-	Favored (70.42%) Glycine / 86.6,11.8	-	-	-	-
A 302	LEU	33.64	0.644Å HD23 with A 200 ILE CD1B	Favored (78.96%) General case / -56.4,-43.0	59.6% ( <i>tp</i> ) chi angles: 176.2,65.3	0.035Å	-	-
A 303	SER	36.1	0.462Å OG A with A 200 ILE HD11A	Favored (26.62%) Pre-proline / -141.2,72.8	70.8% ( <i>p</i> ) chi angles: 57.7	0.013Å	-	-
A 304	PRO	34.1	-	-	83.1% ( <i>Cg_exo</i> ) chi angles: 328.7,44.4,80	0.004Å	-	-
A2001	HOH	28.21	-	-	-	-	-	-
A2002	HOH	35.41	-	-	-	-	-	-
A2003	HOH	30.85	-	-	-	-	-	-
A2004	HOH	49.23	-	-	-	-	-	-
A2005	HOH	49.33	-	-	-	-	-	-
A2006	HOH	44.75	-	-	-	-	-	-

A2007 HOH	53.1	-	-	-	-	-	-
0.503Å							
A2008 HOH	50.35	O with A 54 LYS	-	-	-	-	-
N							
A2009 HOH	50.93	-	-	-	-	-	-
A2010 HOH	42.16	-	-	-	-	-	-
A2011 HOH	31.16	-	-	-	-	-	-
A2012 HOH	35.92	-	-	-	-	-	-
A2013 HOH	52.05	-	-	-	-	-	-

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A2014 HOH	44.23	-	-	-	-	-	-	-
A2015 HOH	33.66	-	-	-	-	-	-	-
A2016 HOH	53.8	-	-	-	-	-	-	-
A2017 HOH	27.67	-	-	-	-	-	-	-
A2018 HOH	22.66	-	-	-	-	-	-	-
A2019 HOH	39.17	-	-	-	-	-	-	-
A2020 HOH	25.21	-	-	-	-	-	-	-
A2021 HOH	39.73	-	-	-	-	-	-	-
A2022 HOH	34.63	-	-	-	-	-	-	-
A2023 HOH	46.92	-	-	-	-	-	-	-
A2024 HOH	36.72	-	-	-	-	-	-	-
A2025 HOH	30.79	-	-	-	-	-	-	-
A2026 HOH	42.89	-	-	-	-	-	-	-
A2027 HOH	44.98	-	-	-	-	-	-	-
A2028 HOH	38.56	-	-	-	-	-	-	-
A2029 HOH	29.97	-	-	-	-	-	-	-
A2030 HOH	28.76	-	-	-	-	-	-	-
A2031 HOH	45.26	-	-	-	-	-	-	-
A2032 HOH	45.98	-	-	-	-	-	-	-
A2033 HOH	41.04	-	-	-	-	-	-	-

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		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A2034 HOH	46.95	-	-	-	-	-	-	-
A2035 HOH	37.54	-	-	-	-	-	-	-
A2036 HOH	44.64	-	-	-	-	-	-	-

A2037 HOH 49.34	-	-	-	-	-	-
A2038 HOH 35.06	-	-	-	-	-	-
A2039 HOH 38.22	-	-	-	-	-	-
A2040 HOH 47.79	-	-	-	-	-	-
A2041 HOH 29.69	-	-	-	-	-	-
A2042 HOH 35.59	-	-	-	-	-	-
A2043 HOH 45.44	-	-	-	-	-	-
A2044 HOH 30.99	-	-	-	-	-	-
A2045 HOH 37.89	-	-	-	-	-	-
A2046 HOH 41.66	-	-	-	-	-	-
A2047 HOH 36.65	-	-	-	-	-	-
A2048 HOH 42.27	-	-	-	-	-	-
A2049 HOH 41.42	-	-	-	-	-	-
A2050 HOH 34.29	-	-	-	-	-	-
A2051 HOH 52.47	-	-	-	-	-	-
A2052 HOH 54.2	-	-	-	-	-	-
A2053 HOH 37.84	-	-	-	-	-	-

#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A2054 HOH 35.51	-	-	-	-	-	-	-	-
A2055 HOH 41.14	-	-	-	-	-	-	-	-
A2056 HOH 43.2	-	-	-	-	-	-	-	-
A2057 HOH 31.35	-	-	-	-	-	-	-	-
A2058 HOH 39.25	-	-	-	-	-	-	-	-
A2059 HOH 35.65	-	-	-	-	-	-	-	-
A2060 HOH 43.68	-	-	-	-	-	-	-	-
A2061 HOH 44.85	-	-	-	-	-	-	-	-
A2062 HOH 25.69	-	-	-	-	-	-	-	-
A2063 HOH 29.74	-	-	-	-	-	-	-	-
A2064 HOH 29.75	-	-	-	-	-	-	-	-
A2065 HOH 32.09	-	-	-	-	-	-	-	-
A2066 HOH 52.61	-	-	-	-	-	-	-	-
A2067 HOH 51.1	-	-	-	-	-	-	-	-
A2068 HOH 37.39	-	-	-	-	-	-	-	-
A2069 HOH 53.92	-	-	-	-	-	-	-	-
A2070 HOH 47.33	-	-	-	-	-	-	-	-
A2071 HOH 40.56	-	-	-	-	-	-	-	-



A2072	HOH	39.9	-	-	-	-	-	-
A2073	HOH	45.2	-	-	-	-	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A2074	HOH	50.08	-	-	-	-	-	-
A2075	HOH	53.5	-	-	-	-	-	-
A2076	HOH	44.9	-	-	-	-	-	-
A2077	HOH	42.18	-	-	-	-	-	-
A2078	HOH	51.54	-	-	-	-	-	-
A2079	HOH	34.67	-	-	-	-	-	-
A2080	HOH	60.42	-	-	-	-	-	-
A2081	HOH	38.49	-	-	-	-	-	-
A2082	HOH	35.32	-	-	-	-	-	-
A2083	HOH	44.42	-	-	-	-	-	-
A2084	HOH	29.47	-	-	-	-	-	-
A2085	HOH	37.29	-	-	-	-	-	-
A2086	HOH	54.81	-	-	-	-	-	-
A2087	HOH	31.68	-	-	-	-	-	-
A2088	HOH	22.67	-	-	-	-	-	-
A2089	HOH	26.58	-	-	-	-	-	-
A2090	HOH	47.01	-	-	-	-	-	-
A2091	HOH	41.63	-	-	-	-	-	-
A2092	HOH	23.22	-	-	-	-	-	-
A2093	HOH	34.32	-	-	-	-	-	-

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		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A2094	HOH	43.81	-	-	-	-	-	-
A2095	HOH	41.29	-	-	-	-	-	-
A2096	HOH	41.7	-	-	-	-	-	-
A2097	HOH	38.53	-	-	-	-	-	-
A2098	HOH	49.2	-	-	-	-	-	-
A2099	HOH	32.77	-	-	-	-	-	-
A2100	HOH	31.79	-	-	-	-	-	-
A2101	HOH	44.33	-	-	-	-	-	-
A2102	HOH	42.87	-	-	-	-	-	-
A2103	HOH	34.18	-	-	-	-	-	-

A2104	HOH	37.17	-	-	-	-	-	-
A2105	HOH	34.1	-	-	-	-	-	-
A2106	HOH	51.79	-	-	-	-	-	-
A2107	HOH	38.71	-	-	-	-	-	-
A2108	HOH	42.92	-	-	-	-	-	-
A2109	HOH	40.89	-	-	-	-	-	-
A2110	HOH	30.9	-	-	-	-	-	-
A2111	HOH	44.77	-	-	-	-	-	-
A2112	HOH	36.97	-	-	-	-	-	-
A2113	HOH	41.86	-	-	-	-	-	-
#	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths.	Bond angles.
		Avg: 33.75	Clashscore: 2.38	Outliers: 0 of 242	Poor rotamers: 0 of 209	Outliers: 0 of 224	Outliers: 0 of 246	Outliers: 1 of 246
A2114	HOH	29.3	-	-	-	-	-	-
A2115	HOH	35.4	-	-	-	-	-	-
A2116	HOH	40.06	-	-	-	-	-	-
A2117	HOH	31.06	-	-	-	-	-	-
A2118	HOH	47.15	-	-	-	-	-	-
A2119	HOH	58.38	-	-	-	-	-	-
A2120	HOH	54.37	-	-	-	-	-	-
A2121	HOH	47.26	-	-	-	-	-	-
A2122	HOH	43.01	-	-	-	-	-	-
A2123	HOH	44.4	-	-	-	-	-	-
A2124	HOH	41.88	-	-	-	-	-	-
A2125	HOH	22.42	-	-	-	-	-	-
A2126	HOH	43.31	-	-	-	-	-	-
A2127	HOH	23.07	-	-	-	-	-	-
A2128	HOH	36.97	-	-	-	-	-	-
A2129	HOH	54	-	-	-	-	-	-
A2130	HOH	36.99	-	-	-	-	-	-
A2131	HOH	52.77	-	-	-	-	-	-
A2132	HOH	44.34	-	-	-	-	-	-
A2133	HOH	20.36	-	-	-	-	-	-
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A2134	HOH	36.68	-	-	-	-	-	-
A2135	HOH	26.32	-	-	-	-	-	-

A2136 HOH 33.53	-	-	-	-	-	-
A2137 HOH 39.48	-	-	-	-	-	-
A2138 HOH 28.82	-	-	-	-	-	-
A2139 HOH 19.32	-	-	-	-	-	-
A2140 HOH 41.32	-	-	-	-	-	-
A2141 HOH 25.61	-	-	-	-	-	-
A2142 HOH 27.01	-	-	-	-	-	-
A2143 HOH 57.85	-	-	-	-	-	-
A2144 HOH 47.92	-	-	-	-	-	-
A2145 HOH 24.54	-	-	-	-	-	-
A2146 HOH 37.37	-	-	-	-	-	-
A2147 HOH 17.93	-	-	-	-	-	-
A2148 HOH 18.19	-	-	-	-	-	-
A2149 HOH 32.59	-	-	-	-	-	-
A2150 HOH 47.08	-	-	-	-	-	-
A2151 HOH 33.76	-	-	-	-	-	-
A2152 HOH 37.63	-	-	-	-	-	-
A2153 HOH 56.41	-	-	-	-	-	-

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A2154 HOH 50.14	-	-	-	-	-	-	-	-
A2155 HOH 53.58	-	-	-	-	-	-	-	-
A2156 HOH 50.09	-	-	-	-	-	-	-	-
A2157 HOH 32.85	-	-	-	-	-	-	-	-
A2158 HOH 50.75	-	-	-	-	-	-	-	-
A2159 HOH 47.53	-	-	-	-	-	-	-	-
A2160 HOH 38.23	-	-	-	-	-	-	-	-
A2161 HOH 38.71	-	-	-	-	-	-	-	-
A2162 HOH 48.35	-	-	-	-	-	-	-	-
A2163 HOH 30.55	-	-	-	-	-	-	-	-
A2164 HOH 32.65	-	-	-	-	-	-	-	-
A2165 HOH 31.73	-	-	-	-	-	-	-	-
A2166 HOH 48.12	-	-	-	-	-	-	-	-
A2167 HOH 30.04	-	-	-	-	-	-	-	-
A2168 HOH 42.42	-	-	-	-	-	-	-	-
A2169 HOH 21.26	-	-	-	-	-	-	-	-
A2170 HOH 28.29	-	-	-	-	-	-	-	-
A2171 HOH 30.51	-	-	-	-	-	-	-	-

A2172	HOH	35.42	-	-	-	-	-	-
A2173	HOH	49.73	-	-	-	-	-	-
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A2174	HOH	35.68	-	-	-	-	-	-
A2175	HOH	25.03	-	-	-	-	-	-
A2176	HOH	20.1	-	-	-	-	-	-
A2177	HOH	21.15	-	-	-	-	-	-
A2178	HOH	25.5	-	-	-	-	-	-
A2179	HOH	42.01	-	-	-	-	-	-
A2180	HOH	43.13	-	-	-	-	-	-
A2181	HOH	22.26	-	-	-	-	-	-
A2182	HOH	19.59	-	-	-	-	-	-
A2183	HOH	15.66	-	-	-	-	-	-
A2184	HOH	30.66	-	-	-	-	-	-
1	UNK	0	-	-	-	-	-	-